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Ab initio studies of electron correlation effects in the atomic parity violating amplitudes in Cs and Fr

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We have studied the correlation effects in Cs and Fr arising from the interplay of the residual Coulomb interaction to all orders and the neutral weak interaction which gives rise to the parity violating electric dipole transition to first order, within the framework of the relativistic coupled-cluster theory which circumvents the constrain of explicitly summing over the intermediate states. We observe that, the contributions arising from the perturbed doubly excited states are quite significant and hence, any calculation should not be considered accurate unless it includes the perturbed double excitations comprehensively. In this article, we have reported a comparative study of various results related to the parity violation in Cs and Fr.

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Keywords: atomic parity violation, ab initio method, coupled-cluster theory

I. INTRODUCTION

One of the most challenging contemporary problems in physics is the search for possible new physics beyond the well known standard model (SM) of elementary particles [1–4]. Apart from using gigantic accelerators at high-energy scales, it is also possible to use high precision, albeit, low-energy table top atomic experiments, such as, the measurement of atomic parity violation, in combination with accurate relativistic many-body calculations of the atomic parity nonconserving transition amplitude, E_{1PNC} to achieve this goal [4, 5]. Some of the prominent signatures of physics beyond the SM which can be inferred from these atomic experiments are: a tight limit on the mass of extra Z-bosons, precise value of the Weinberg angle, limit to the radiative corrections for the electron-nuclear weak interactions etc [4]. As some of these SM results are known to high precision, they demand similar sub-one percent accuracies in both the measurements and the atomic calculations. As the interaction Hamiltonian for the atomic parity violation (APV) due to the nuclear spin-independent (NSI) electron-nucleus interactions is proportional to Z^3 where Z being the atomic number [5], heavy atomic systems are chosen for the study of APV effects. A series of APV experiments on a number of atomic systems, including those of Cs [6] and Tl [7] have been carried out. However, the high accuracy of $\sim 0.35\%$ has been achieved only for Cs. Furthermore, a number of ab initio calculations of APV amplitudes in Cs have been carried out using a variety of many-body approaches. Some results based on the relativistic coupled-cluster (RCC) theory are also available for Cs, however, their accuracies are somewhat uncertain, since most of them have used the sum-over-states approach which considers contributions from the core orbitals approximately and accounts for only a selected number of excited states whose contributions are dominant. In addition, the doubly excited intermediate atomic states and the normalization of the RCC wave functions are treated only approximately. We have developed a technique in the frame work of RCC theory that circumvents these drawbacks and it has been employed earlier in the calculation of the E_{1PNC} amplitudes in Ba^+ [8] and Ra^+ [9] in which we have demonstrated that the accuracies of $< 1\%$ and $< 3\%$, respectively, were possible.

In this work, we employ the new RCC approach, mentioned above, to study various correlation effects in the parity violating amplitudes in Cs and Fr. We report a comparative study of their results along with those reported previously.

II. THEORY OF APV

The dominant interaction in an atom is the electromagnetic interaction which, as well known, conserves parity. However, there is a non-zero probability of the interaction between the electrons and the nucleus of an atom due to the weak force with the exchange of a Z_0 boson, as shown in Fig. 1, which violates parity. The interaction Hamiltonian between the electrons and the nucleus due to the weak interaction can have two components: one, vector–axial-vector and the other, axial-vector–vector currents. The latter depends on the nuclear spin and most of its contribution cancels out except from the odd nucleon and hence, it is relatively smaller in magnitude [5] than the former; the NSI component. In this work, we shall consider the APV effect due to the NSI component alone.

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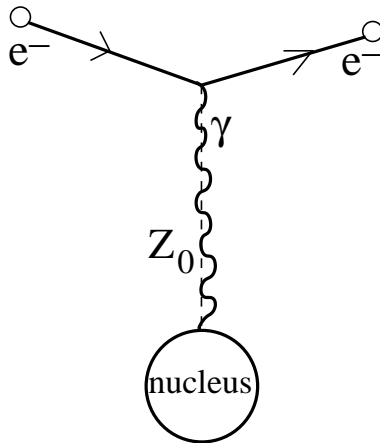


FIG. 1: Diagrammatic representation of the electron-nucleus interactions due to the electromagnetic (with the exchange of photon γ denoted by solid curved line) and the weak (with the exchange of heavy boson Z_0 denoted by straight dashed line) interactions.

The APV interaction Hamiltonian due to the NSI component is given by,

$$H_{APV}^{NSI} = \frac{G_F}{2\sqrt{2}} Q_w(N) \gamma_5^e \rho_N^e(r), \quad (2.1)$$

where G_F is the Fermi constant, $\rho_N^e(r)$ is the electron density over the nucleus and $\gamma_5^e (= i\gamma_0^e \gamma_1^e \gamma_2^e \gamma_3^e)$, is the product of the four Dirac matrices that involve electron spin, and $Q_w(N)$ is the nuclear weak charge, which is equal to $2(Zc_p + Nc_n)$ where c_p and c_n denote the electron-proton and the electron-neutron coupling constants for the atomic (Z) and neutron (N) numbers, respectively. The values of these coupling constants predicted by the SM, in the lowest order of electroweak interaction (at the tree level), are given by

$$c_p = \frac{1}{2}(1 - 4\sin^2\theta_W) \approx 0.04, \quad c_n = -\frac{1}{2}, \quad (2.2)$$

where θ_W is the Weinberg angle and its measured value is $\sim \sin^2\theta_W \approx 0.23$ [10]. Substituting these values in $Q_w(N)$, we get $Q_w(N) = -N + Z(1 - \sin^2\theta_W)$ which is proportional to N . Hence, the perturbation due to H_{APV}^{NSI} is generally expressed in the scale of $Q_w(N)/N$. Since H_{APV}^{NSI} does not commute with the parity operator, its inclusion with the atomic Hamiltonian of the electromagnetic interaction, which commutes with the parity operator, mixes the opposite parity states of same angular momentum. The strength of this interaction is sufficiently weak, which justifies its consideration as a first-order perturbation.

The Dirac-Coulomb (DC) Hamiltonian used, here, in the calculation of the atomic wave functions of definite parity is given by

$$H^{DC} = \sum_i [c\alpha \cdot p_i + (\beta - 1)c^2 + V_{nuc}(r_i)] + \sum_{i>j} \frac{1}{r_{ij}}, \quad (2.3)$$

where c is the velocity of light, α and β are the Dirac matrices (note that $\gamma^e = \beta\alpha$) and $V_{nuc}(r)$ is the nuclear potential.

The atomic wave functions ($|\Psi_n^{(0)}\rangle$) corresponding to H^{DC} can be considered as the unperturbed wave functions. The total wave function of a system including the first order correction due to the interaction Hamiltonian H_{APV}^{NSI} is given by

$$|\Psi_n\rangle = |\Psi_n^{(0)}\rangle + G_F |\Psi_n^{(1)}\rangle, \quad (2.4)$$

where $|\Psi_n^{(1)}\rangle$ is the first order perturbed wave function of its unperturbed valence state $|\Psi_n^{(0)}\rangle$ and G_F is used as a coupling constant.

Electric dipole (E1) transitions between the states of same parity are forbidden due to the electromagnetic selection rules. However, an E1 transition between the states of mixed parity, mixed due to H_{APV}^{NSI} interaction, is possible and

the corresponding transition amplitude can be expressed as

$$E1_{PNC} = \frac{\langle \Psi_f | D | \Psi_i \rangle}{\sqrt{\langle \Psi_f | \Psi_f \rangle \langle \Psi_i | \Psi_i \rangle}}, \quad (2.5)$$

where $D = er$ is the E1 operator, the subscripts i and f denote initial and final valence orbitals, respectively.

Expanding the total wave function as given in Eq. (2.4) and retaining the terms only up to first order in G_F , we get

$$\begin{aligned} E1_{PNC} &= G_F \frac{\langle \Psi_f^{(0)} | D | \Psi_i^{(1)} \rangle + \langle \Psi_f^{(1)} | D | \Psi_i^{(0)} \rangle}{\sqrt{\langle \Psi_f^{(0)} | \Psi_f^{(0)} \rangle \langle \Psi_i^{(0)} | \Psi_i^{(0)} \rangle}} \\ &= G_F \sum_{I \neq i} \frac{\langle \Psi_f^{(0)} | D | \Psi_I^{(0)} \rangle \langle \Psi_I^{(0)} | H_{APV}^{NSI} | \Psi_i^{(0)} \rangle}{E_i - E_I} \\ &\quad + G_F \sum_{J \neq f} \frac{\langle \Psi_f^{(0)} | H_{APV}^{NSI} | \Psi_J^{(0)} \rangle \langle \Psi_J^{(0)} | D | \Psi_i^{(0)} \rangle}{E_f - E_J}, \end{aligned} \quad (2.6)$$

where the subscripts I and J represent the intermediate unperturbed states. We have used, here, the explicit form for the first order wave function given by

$$|\Psi_n^{(1)}\rangle = \frac{1}{G_F} \sum_{I \neq n} |\Psi_I^{(0)}\rangle \frac{\langle \Psi_I^{(0)} | H_{APV}^{NSI} | \Psi_n^{(0)} \rangle}{E_n - E_I}. \quad (2.7)$$

An important question we address in this paper is: How significant are the contributions from those states which were considered approximately in the sum-over-states approach and how they vary with the size of the systems? We would address this by carrying out a comparative study of $E1_{PNC}$ results in two systems, namely Cs and Fr, of different atomic sizes. In order for the contributions of these higher excited states to be included, it is necessary to solve the first order perturbation equation directly. In other words, it is necessary to solve the equation following equation

$$(H^{DC} - E^{(0)})|\Psi_n^{(1)}\rangle = \frac{1}{G_F}(E^{(1)} - H_{APV}^{NSI})|\Psi_n^{(0)}\rangle, \quad (2.8)$$

where $E^{(1)} (= \langle \Psi_n^{(0)} | H_{APV}^{NSI} | \Psi_n^{(0)} \rangle)$ is the first order correction to $E^{(0)}$ which, however, vanishes in the present case.

III. APPLICATION OF RCC THEORY TO APV

The RCC method, which is equivalent to all order perturbation theory, has been used in the recent past and accurate results have been reported for many single valence systems [8, 9, 11, 12]. In the RCC framework, the wave function of a single valence atom can be expressed as

$$|\Psi_n^{(0)}\rangle = e^{T^{(0)}} \{1 + S_n^{(0)}\} |\Phi_n\rangle, \quad (3.1)$$

where $|\Phi_n\rangle$ is the reference state constructed from the Dirac-Fock (DF) wave function $|\Phi_0\rangle$ of the closed-shell configuration by appending the valence electron n , that is, $|\Phi_n\rangle = a_n^\dagger |\Phi_0\rangle$ where a_n^\dagger represents a creation operator which creates the valence electron n . Here $T^{(0)}$ and $S_n^{(0)}$ are the RCC excitation operators which excite electrons from $|\Phi_0\rangle$ and $|\Phi_n\rangle$, respectively, due to the residual Coulomb interactions. The corresponding excitation amplitudes are obtained by solving the following equations

$$\langle \Phi^L | \{ \widehat{H_N^{DC}} e^{\widehat{T^{(0)}}} \} | \Phi_0 \rangle = 0 \quad (3.2)$$

$$\langle \Phi_n^L | \{ \widehat{H_N^{DC}} e^{\widehat{T^{(0)}}} \} S_n | \Phi_n \rangle = - \langle \Phi_n^L | \{ \widehat{H_N^{DC}} e^{\widehat{T^{(0)}}} \} | \Phi_n \rangle + \langle \Phi_n^L | S_n | \Phi_n \rangle \Delta E_n^{(0)}, \quad (3.3)$$

with the superscript $L (= 1, 2)$ representing the singly and doubly excited states from the corresponding reference states and the wide-hat symbol over $H_N^{DC} e^{T^{(0)}}$ represent the linked terms of normal order atomic Hamiltonian H_N^{DC}

and RCC operator $T^{(0)}$. In the CCSD (CC with single and double excitations) approximation, the corresponding RCC operators are defined by

$$T^{(0)} = T_1^{(0)} + T_2^{(0)} \quad (3.4)$$

and

$$S_n^{(0)} = S_{1n}^{(0)} + S_{2n}^{(0)} \quad (3.5)$$

for the closed-shell and single valence open-shell systems, respectively. The quantity $\Delta E_n^{(0)}$ in the above expression is the electron affinity energy (or negative of the ionization potential (IP)) for the valence electron which is evaluated by

$$\Delta E_n^{(0)} = \langle \Phi_n | \{ \widehat{H_N^{DC}} e^{T^{(0)}} \} \{ 1 + S_n^{(0)} \} | \Phi_n \rangle. \quad (3.6)$$

In addition to having considered full singles and doubles in the CCSD equations given in Eq. (3.3), we have also included the contributions from the important triple excitations perturbatively (known in the literature as CCSD(T) method) by defining

$$S_{3n}^{(0),pert} = \widehat{H_N^{DC}} T_2^{(0)} + \widehat{H_N^{DC}} S_{2n}^{(0)}, \quad (3.7)$$

where the superscript *pert* denotes the perturbation and their contributions to $\Delta E_n^{(0)}$ are evaluating as

$$\Delta E_n^{(0),trip} = T_2^{(0)\dagger} \widehat{S_{3n}^{(0),pert}}. \quad (3.8)$$

After solving for the amplitudes of $T^{(0)}$, we solve Eqs. (3.3) and (3.6) simultaneously and obtain the amplitudes of $S_n^{(0)}$ operators.

Now, the total atomic wave function in the presence of H_{APV}^{NSI} is expressed, in the RCC ansatz, as

$$|\Psi_n\rangle = e^{T^{(0)} + G_F T^{(1)}} \{ 1 + S_n^{(0)} + G_F S_n^{(1)} \} |\Phi_n\rangle, \quad (3.9)$$

where $T^{(1)}$ and $S_n^{(1)}$ are the first order perturbed amplitudes corresponding to the unperturbed RCC operators $T^{(0)}$ and $S_n^{(0)}$, respectively. On expanding the above equation keeping the terms only up to first order in G_F yields

$$|\Psi_n\rangle = e^{T^{(0)}} \{ 1 + S_n^{(0)} + G_F T^{(1)} (1 + S_n^{(0)}) + G_F S_n^{(1)} \} |\Phi_n\rangle. \quad (3.10)$$

Comparing the above equation with Eq. (2.4), we get

$$|\Psi_n^{(1)}\rangle = e^{T^{(0)}} \{ T^{(1)} (1 + S_n^{(0)}) + S_n^{(1)} \} |\Phi_n\rangle. \quad (3.11)$$

In order to calculate $|\Psi_n^{(1)}\rangle$ as a solution of Eq. (2.8) in the RCC theory, we solve the excitation operator amplitudes of $T^{(1)}$ and $S_n^{(1)}$ using the following equations

$$\langle \Phi^L | \{ \widehat{H_N^{DC}} e^{T^{(0)}} T^{(1)} \} | \Phi_0 \rangle = - \langle \Phi^L | \widehat{H_{APV}^{NSI}} e^{T^{(0)}} | \Phi_0 \rangle \quad (3.12)$$

and

$$\begin{aligned} \langle \Phi_n^L | \{ \widehat{H_N^{DC}} e^{T^{(0)}} \} S_n^{(1)} | \Phi_n \rangle &= - \langle \Phi_n^L | \{ \widehat{H_N^{DC}} e^{T^{(0)}} T^{(1)} (1 + S_n^{(0)}) \\ &\quad + \widehat{H_{APV}^{NSI}} e^{T^{(0)}} (1 + S_n^{(0)}) \} | \Phi_n \rangle + \langle \Phi_n^L | S_n^{(1)} | \Phi_n \rangle \Delta E_n, \end{aligned} \quad (3.13)$$

after solving Eq. (3.2) and Eq. (3.3), respectively. In the above expression, notation $\widehat{H_{APV}^{NSI}} e^{T^{(0)}}$ is used for the connecting terms between $\widehat{H_{APV}^{NSI}}$ and $T^{(0)}$. To keep the level of approximation uniform through out, both $T^{(1)}$ and $S_n^{(1)}$ are truncated at single and double excitations by defining

$$T^{(1)} = T_1^{(1)} + T_2^{(1)} \quad (3.14)$$

and

$$S_n^{(1)} = S_{1n}^{(1)} + S_{2n}^{(1)} \quad (3.15)$$

where $T_1^{(1)}$ and $S_{1n}^{(1)}$ correspond to the perturbed single excitations and $T_2^{(1)}$ and $S_{2n}^{(1)}$ correspond to the perturbed double excitations, from closed- and open-shells, respectively. Since both the perturbed single and double excitation amplitudes are solved simultaneously, certain correlation effects due to the perturbed double excitations also reflect indirectly in the contributions of the perturbed single excitations.

After obtaining the unperturbed and the perturbed RCC operator amplitudes in both the closed-shell and one-valence open-shell atoms, we proceed to calculate the $E1_{PNC}$ amplitude as

$$\begin{aligned} E1_{PNC} &= G_F \frac{\langle \Psi_n^{(0)} | D | \Psi_n^{(1)} \rangle + \langle \Psi_n^{(1)} | D | \Psi_n^{(0)} \rangle}{\langle \Psi_n^{(0)} | \Psi_n^{(0)} \rangle} \\ &= G_F \frac{\langle \Phi_n | \{1 + S_n^{(0)\dagger}\} \overline{D} \{T_1^{(1)}(1 + S_n^{(0)}) + S_{1n}^{(1)}\} | \Phi_n \rangle}{\langle \Phi_n | \{1 + S_n^{(0)\dagger}\} \overline{N}_0 \{1 + S_n^{(0)}\} | \Phi_n \rangle} \\ &\quad + G_F \frac{\langle \Phi_n | \{S_n^{(1)\dagger} + (1 + S_n^{(0)\dagger})T_1^{(1)\dagger}\} \overline{D} \{1 + S_n^{(0)}\} | \Phi_n \rangle}{\langle \Phi_n | \{1 + S_n^{(0)\dagger}\} \overline{N}_0 \{1 + S_n^{(0)}\} | \Phi_n \rangle}, \end{aligned} \quad (3.16)$$

where we define $\overline{D} = (e^{T^{(0)\dagger}} D e^{T^{(0)}})$ and $\overline{N}_0 = e^{T^{(0)\dagger}} e^{T^{(0)}}$. The non-truncative series for \overline{D} and \overline{N}_0 are expanded using the Wick's generalized theorem and are truncated when the terms are below fifth order of the Coulomb interaction. The core-valence and valence correlation contributions are obtained from $DT_1^{(1)}$ and $D(T_1^{(1)}\{1 + S_n^{(0)}\} + S_{1n}^{(1)})$, respectively, along with their conjugate terms.

Corrections due to the normalization of the wave functions are accounted by evaluating

$$Norm = \left[\langle \Psi_n^{(0)} | D | \Psi_n^{(1)} \rangle + \langle \Psi_n^{(1)} | D | \Psi_n^{(0)} \rangle \right] \left\{ \frac{N_n}{1 + N_n} \right\}, \quad (3.17)$$

where $N_n = \langle \Phi_n | \{1 + S_n^{(0)\dagger}\} \overline{N}_0 \{1 + S_n^{(0)}\} | \Phi_n \rangle$.

Although, the CCSD(T) method described here, accounts for the contributions from the important unperturbed triple excitations it fails to include the direct triple excitation contributions to the $E1_{PNC}$ calculations. To account for, at least, the lowest order direct triple excitation contributions (minimum up to fourth order in Coulomb interaction), we construct them with the open-shell RCC operators perturbatively as follows

$$S_{nab}^{pqr,(0)} = \frac{\widehat{H_N^{DC} T_2^{(0)}} + \widehat{H_N^{DC} S_{2n}^{(0)}}}{\epsilon_n + \epsilon_a + \epsilon_b - \epsilon_p - \epsilon_q - \epsilon_r}, \quad (3.18)$$

and

$$S_{nab}^{pqr,(1)} = \frac{\widehat{H_N^{DC} T_2^{(1)}} + \widehat{H_N^{DC} S_{2n}^{(1)}}}{\epsilon_n + \epsilon_a + \epsilon_b - \epsilon_p - \epsilon_q - \epsilon_r}, \quad (3.19)$$

where ϵ_i is the single particle energy of an orbital i . These operators are finally considered as parts of $S_n^{(0)}$ and $S_n^{(1)}$ in Eq. (III). This can be called as lo-CCSDvT approximation, which also accounts important lower order valence triple excitation effects in the final property calculations.

IV. RESULTS AND DISCUSSIONS

A. Orbitals generation

We have used Gaussian type functions

$$F^{GTO}(r_i) = r_i^{n_\kappa} e^{-\alpha_i r_i^2} \quad (4.1)$$

to construct the DF orbitals where α_i is an arbitrary parameter which has to be chosen and r_i represents a radial grid given by

$$r_i = r_0 \left[e^{h(i-1)} - 1 \right] \quad (4.2)$$

where the step size h is taken to be 0.03, the radial grid is increased up to $i = 750$, r_0 is 2×10^{-6} in atomic units and n_κ is the radial quantum number of the orbitals. Here α_i s are chosen to satisfy the even tempering condition

$$\alpha_i = \alpha_0 \beta^{i-1} \quad (4.3)$$

and we have chosen different α_0 and β values for different symmetries (l) (known as even tempered basis) and they are given in Table I.

TABLE I: Used α_0 and β parameters for different symmetries (l) to construct DF orbitals using GTOs in Cs and Fr.

α_0/β \backslash l	0	1	2	3	4
α_0	0.00190	0.001825	0.00183	0.00185	0.00187
β	2.91	2.94	2.94	3.05	3.09

The finite size of the nucleus in these systems is accounted by assuming a two-parameter Fermi-nuclear-charge distribution for evaluating the electron density over the nucleus as given by

$$\rho(r_i) = \frac{\rho_0}{1 + e^{(r_i-c)/a}}, \quad (4.4)$$

where ρ_0 is the density for the point nuclei, c and a are the half-charge radius and skin thickness of the nucleus. These parameters are chosen as

$$a = 2.3/4(\ln 3) \quad (4.5)$$

and

$$c = \sqrt{\frac{5}{3}r_{rms}^2 - \frac{7}{3}a^2\pi^2}, \quad (4.6)$$

where r_{rms} is the root mean square radius of the corresponding nuclei which is determined by

$$r_{rms} = 0.836A^{1/3} + 0.570 \quad (4.7)$$

in fm for the atomic mass A .

B. Results

In Table II, we give the $E1_{PNC}$ amplitude results obtained from various calculations. From this work, we present the results using the DF, CCSD, CCSD(T) and lo-CCSDvT methods for both Cs and Fr. In the same table, we also compare our results with previously reported results using various many-body methods. Our Cs result matches reasonably well with the other calculations, but our Fr result differs significantly. We give below individual contributions from various RCC terms and express them in terms of correlation diagrams and level of excitations in order to facilitate the readers to understand the role of various correlation effects and intermediate states. Briefly, we discuss here the methods used in the other calculations. The difference between our DF and lo-CCSDvT results gives an idea about the amount of total correlation effects through the present method in these calculations. Considering the same DF wave functions, we have also employed CCSD and CCSD(T) methods where we find that the CCSD results are larger in magnitude than the CCSD(T) results. However, the $E1_{PNC}$ result increases in magnitude for Cs in the lo-CCSDvT approximation, but it decreases for Fr; indicating that the triple excitation effects are stronger in Fr. From a comparison between these results, we observe that the dominant triple excitations effects arise through the CCSD(T) method.

TABLE II: Comparison of $E1_{PNC}$ results of ^{133}Cs and ^{223}Fr due to electron-electron Coulomb interactions from various methods in $\times 10^{-11} iea_0(-Q_W/N)$.

^{133}Cs	^{223}Fr	Method	Reference
$6s\ ^2S_{1/2} \rightarrow 7s\ ^2S_{1/2}$	$7s\ ^2S_{1/2} \rightarrow 8s\ ^2S_{1/2}$		
-0.7236	-13.4825	DF	This work
-0.8941	-14.5134	CCSD	This work
-0.8889	-14.4219	CCSD(T)	This work
-0.8892	-14.4106	lo-CCSDvT	This work
-0.904(9)		LCCSD(T) + SL + SS	[13]
-0.9078		BO + GFCP	[14]
-0.904	-15.72	CI	[15]
-0.902(4)		CCSD(T)	[16]
-0.9001	-15.229	BO + GFCP	[17]
-0.8998(25)		CCSDvT + SS	[18]
	-15.9	BO + GFCP	[19]
	-15.41(17)	LCCSD + RPA + ExpEng + SS	[20]

NOTE: Contributions from Breit interaction, QED correction and nuclear effects are not considered here.

Abbreviations	SS	: sum-over-states
	SL	: scaling
	BO	: Brueckner orbitals
	GFCP	: Green function technique for all order correlation potential
	CI	: configuration interaction method
	ExpEng	: experimental energy
	RPA	: random phase approximation

C. Discussions

Here we discuss briefly different reported calculations of the above results at the DC approximation. About two decades ago, Blundell et al [13] had employed the linearized CCSD(T) method (LCCSD(T) method) to evaluate the unperturbed wave functions in Cs and then they had used a sum-over-states approach to evaluate the $E1_{PNC}$ amplitude for the $6s\ ^2S_{1/2} \rightarrow 7s\ ^2S_{1/2}$ transition in Cs. However, they had scaled their wave functions to fit the calculated energies of different states with the experimental results which reproduced many atomic properties quite accurately, but that does not show that the method they had used is capable of producing accurate ab initio results. Shabaev et al [15] have also obtained results using a CI method with a local form of the DF wave functions. Their Cs result matches with the result of Blundell et al. In our previous work on Cs [16], we had also calculated this quantity by considering the same α_0 and β parameters for orbitals of all symmetries (known as universal basis). With the new parameters, the Gaussian basis orbitals produce better wave functions in the nuclear region which are verified by studying the hyperfine interactions that will be reported elsewhere. The convergence of the RCC amplitudes are better than 10^{-8} in the present case than 10^{-6} in [16] and it gives a slightly different result. Dzuba et al have carried out a few calculations of these quantities using Brueckner orbitals using a Green function technique (Feynman diagram approach) that takes into account various classes of correlation effects to all orders and avoids the sum-over-states approach [14, 17, 19]. Their results also differ from each other and in some cases with others as can be seen in Table I. The most recent calculation on Cs is reported by Porsev et al [18] using the RCC method that includes all single and double excitations with all valence triple excitations (CCSDvT method). However, they have finally used a sum-over-states approach to calculate the $E1_{PNC}$ amplitude of the $6s\ ^2S_{1/2} \rightarrow 7s\ ^2S_{1/2}$ transition. They give contributions from $6p_{1/2}$ to $9p_{1/2}$ singly excited states as "Main", which contributes $-0.8823(18)$, and the remaining contributions as "Tail", which is obtained using other many-body methods as $-0.0175(18)$, (results are always given in $\times 10^{-11} iea_0(-Q_W/N)$ here onwards) at the DC approximation. In contrast to their approach, we have used the lo-CCSDvT method, but have included contributions from the core and doubly excited states in a manner similar to that of the singly excited states.

TABLE III: Contributions to the $E1_{PNC}$ calculations in Cs and Fr using CCSD(T) method (in $\times 10^{-11}iea_0(-Q_W/N)$).

(A) Cs			
Initial pert. terms ($6s^2S_{1/2}^{(1)} \rightarrow 7s^2S_{1/2}^{(0)}$)		Final pert. terms ($6s^2S_{1/2}^{(0)} \rightarrow 7s^2S_{1/2}^{(1)}$)	
DF result			
DH_{APV}^{NSI}	-1.0460	$H_{APV}^{NSI}D$	0.3224
$T_1^{(1)\dagger}D$	0.0374	$DT^{(1)}$	-0.0355
$\overline{D}_1S_{1i}^{(1)}$	-1.7467	$S_{1f}^{(1)\dagger}\overline{D}_1$	0.1841
$\overline{D}_1S_{2i}^{(1)}$	-0.0046	$S_{2f}^{(1)\dagger}\overline{D}_1$	0.0226
$S_{1f}^{(0)\dagger}\overline{D}_1S_{1i}^{(1)}$	0.4061	$S_{1f}^{(1)\dagger}\overline{D}_1S_{1i}^{(0)}$	0.2141
$S_{2f}^{(0)\dagger}\overline{D}_1S_{1i}^{(1)}$	-0.0055	$S_{1f}^{(1)\dagger}\overline{D}_1S_{2i}^{(0)}$	0.0301
$S_{1f}^{(0)\dagger}\overline{D}_1S_{2i}^{(1)}$	-0.0026	$S_{2f}^{(1)\dagger}\overline{D}_1S_{1i}^{(0)}$	-0.0028
$S_{2f}^{(0)\dagger}\overline{D}_1S_{2i}^{(1)}$	0.0011	$S_{2f}^{(1)\dagger}\overline{D}_1S_{2i}^{(0)}$	-0.0073
<i>Others</i>	-0.0045		0.0054
<i>Norm</i>	0.0301		-0.0105
(B) Fr			
Initial pert. terms ($7s^2S_{1/2}^{(1)} \rightarrow 8s^2S_{1/2}^{(0)}$)		Final pert. terms ($7s^2S_{1/2}^{(0)} \rightarrow 8s^2S_{1/2}^{(1)}$)	
DF result			
DH_{APV}^{NSI}	-19.4661	$H_{APV}^{NSI}D$	5.9836
$T_1^{(1)\dagger}D$	0.7147	$DT^{(1)}$	-0.6876
$\overline{D}_1S_{1i}^{(1)}$	-31.7107	$S_{1f}^{(1)\dagger}\overline{D}_1$	4.0538
$\overline{D}_1S_{2i}^{(1)}$	-0.0314	$S_{2f}^{(1)\dagger}\overline{D}_1$	0.5930
$S_{1f}^{(0)\dagger}\overline{D}_1S_{1i}^{(1)}$	7.8001	$S_{1f}^{(1)\dagger}\overline{D}_1S_{1i}^{(0)}$	4.1072
$S_{2f}^{(0)\dagger}\overline{D}_1S_{1i}^{(1)}$	-0.0423	$S_{1f}^{(1)\dagger}\overline{D}_1S_{2i}^{(0)}$	0.6580
$S_{1f}^{(0)\dagger}\overline{D}_1S_{2i}^{(1)}$	-0.0615	$S_{2f}^{(1)\dagger}\overline{D}_1S_{1i}^{(0)}$	-0.0911
$S_{2f}^{(0)\dagger}\overline{D}_1S_{2i}^{(1)}$	0.0033	$S_{2f}^{(1)\dagger}\overline{D}_1S_{2i}^{(0)}$	-0.1501
<i>Others</i>	-0.0152		0.0769
<i>Norm</i>	0.6043		-0.2433

D. Cs vs. Fr

In Table III, we present the individual contributions from different RCC terms in our CCSD(T) method to the $E1_{PNC}$ calculations for the $6s^2S_{1/2} \rightarrow 7s^2S_{1/2}$ and $7s^2S_{1/2} \rightarrow 8s^2S_{1/2}$ transitions in Cs and Fr, respectively. It is evident that the trends of the contributions from the different RCC terms are similar for both Cs and Fr. The important contributions come from three terms: $\overline{D}_1S_{1i}^{(1)}$, $\overline{D}_1S_{2i}^{(1)}$ and $DT_1^{(1)}$ and their corresponding conjugate terms where \overline{D}_1 is the effective one-body terms of \overline{D} and bare operator D is its lowest order term. Other terms correspond to higher order RCC terms, but they are not small. Contributions given as *Others* represent the RCC terms that come from the effective two-body terms of \overline{D} after contracting with the open-shell RCC terms. We give diagrammatic representations of the above three RCC terms in Fig 2 (without their conjugate terms) and their lowest order terms. From this figure, it can be noticed that $DT_1^{(1)}$ and $\overline{D}_1S_{1i}^{(1)}$ contain the lowest order DF contributions from the core (hole) and virtual orbitals, respectively; hence $\overline{D}_1S_{1i}^{(1)}$ always gives the largest contribution. Again, the perturbed states arising through the ground state contribute predominantly while contributions from the perturbed excited states are comparatively smaller than those corresponding to the ground state but with the opposite signs. The final results are the outcome of these cancellations. The most core correlation effects are coming from $DT_1^{(1)}$ and its conjugate terms while there are small contributions that come from $\overline{D}_1S_{2i}^{(1)}$ and its conjugate terms which are included in "Others". As seen these correlation effects mostly cancel out with their corresponding conjugate terms in both the systems. The contributions from singly excited states can be estimated by summing the total contributions from $\overline{D}_1S_{1i}^{(1)}$, $S_{1f}^{(0)\dagger}\overline{D}_1S_{1i}^{(1)}$, $S_{2f}^{(0)\dagger}\overline{D}_1S_{1i}^{(1)}$ and their conjugate RCC terms. The remaining contributions are come from the doubly excited states apart from the normalization corrections to the RCC wave functions. After accounting the

TABLE IV: Important contributions to the $E1_{PNC}$ calculations in Cs from various intermediate states (I and J notations are used as per Eq. (2.6) in $\times 10^{-11}iea_0(-Q_W/N)$).

$6s^2\bar{S}_{1/2}^{(1)} \rightarrow 7s^2\bar{S}_{1/2}^{(0)}$		$6s^2\bar{S}_{1/2}^{(0)} \rightarrow 7s^2\bar{S}_{1/2}^{(1)}$		
I	Results	J	Results	
$T_1^{(1)\dagger}D$		$DT^{(1)}$		
	$4p_{1/2} \rightarrow 7s$	0.0005	$4p_{1/2} \rightarrow 6s$	-0.0005
	$5p_{1/2} \rightarrow 7s$	0.0368	$5p_{1/2} \rightarrow 6s$	-0.0349
$\bar{D}_1S_{1i}^{(1)}$		$S_{1f}^{(1)\dagger}\bar{D}_1$		
	$6s \rightarrow 6p_{1/2}$	-1.9195	$7s \rightarrow 6p_{1/2}$	1.7648
	$6s \rightarrow 7p_{1/2}$	0.1532	$7s \rightarrow 7p_{1/2}$	-1.5022
	$6s \rightarrow 8p_{1/2}$	0.0347	$7s \rightarrow 8p_{1/2}$	-0.0902
	$6s \rightarrow 9p_{1/2}$	-0.0084	$7s \rightarrow 10p_{1/2}$	0.0093
	$6s \rightarrow 10p_{1/2}$	-0.0051		
$S_{1f}^{(0)\dagger}\bar{D}_1S_{1i}^{(1)}$		$S_{1f}^{(1)\dagger}\bar{D}_1S_{1i}^{(0)}$		
	$6s \rightarrow 6p_{1/2}$	0.1716	$7s \rightarrow 6p_{1/2}$	0.2556
	$6s \rightarrow 7p_{1/2}$	0.1302	$7s \rightarrow 7p_{1/2}$	0.1213
	$6s \rightarrow 8p_{1/2}$	0.0258	$7s \rightarrow 8p_{1/2}$	-0.0611
	$6s \rightarrow 9p_{1/2}$	0.0735	$7s \rightarrow 9p_{1/2}$	-0.0946
	$6s \rightarrow 10p_{1/2}$	0.0053	$7s \rightarrow 10p_{1/2}$	-0.0055
$\bar{D}_1S_{2i}^{(1)}$		$S_{2f}^{(1)\dagger}\bar{D}_1$		
	$6s5p_{1/2} \rightarrow 7s6s$	-0.0019	$7s5p_{3/2} \rightarrow 6s9s$	0.0002
	$6s5p_{1/2} \rightarrow 7s8s$	-0.0001	$7s5p_{3/2} \rightarrow 6s10s$	0.0009
	$6s5p_{3/2} \rightarrow 7s8s$	0.0001	$7s5p_{1/2} \rightarrow 6s6d_{3/2}$	0.0001
	$6s5p_{1/2} \rightarrow 7s9s$	-0.0009	$7s5p_{3/2} \rightarrow 6s6d_{3/2}$	-0.0003
	$6s5p_{3/2} \rightarrow 7s9s$	0.0009	$7s5p_{3/2} \rightarrow 6s7d_{3/2}$	-0.0001
	$6s5p_{1/2} \rightarrow 7s10s$	-0.0014	$7s5p_{1/2} \rightarrow 6s8d_{3/2}$	0.0006
	$6s5p_{3/2} \rightarrow 7s10s$	0.0001	$7s5p_{3/2} \rightarrow 6s8d_{3/2}$	-0.0003
	$6s5s \rightarrow 7s9p_{1/2}$	0.0001	$7s5p_{1/2} \rightarrow 6s9d_{3/2}$	0.0019
	$6s5s \rightarrow 7s10p_{1/2}$	0.0002	$7s5p_{3/2} \rightarrow 6s9d_{3/2}$	0.0003
	$6s5p_{1/2} \rightarrow 7s6d_{3/2}$	0.0006	$7s5p_{1/2} \rightarrow 6s10d_{3/2}$	0.0005
	$6s5p_{3/2} \rightarrow 7s6d_{3/2}$	0.0005	$7s5p_{3/2} \rightarrow 6s10d_{3/2}$	0.0001
	$6s5p_{1/2} \rightarrow 7s7d_{3/2}$	0.0003	$7s5p_{3/2} \rightarrow 6s5d_{5/2}$	0.0044
	$6s5p_{3/2} \rightarrow 7s7d_{3/2}$	0.0002	$7s5p_{3/2} \rightarrow 6s6d_{5/2}$	0.0018
	$6s5p_{1/2} \rightarrow 7s8d_{3/2}$	0.0013	$7s5p_{3/2} \rightarrow 6s7d_{5/2}$	0.0008
	$6s5p_{3/2} \rightarrow 7s8d_{3/2}$	0.0011	$7s5p_{3/2} \rightarrow 6s8d_{5/2}$	0.0041
	$6s5p_{1/2} \rightarrow 7s9d_{3/2}$	0.0006	$7s5p_{3/2} \rightarrow 6s9d_{5/2}$	0.0048
	$6s5p_{3/2} \rightarrow 7s9d_{3/2}$	0.0005	$7s5p_{3/2} \rightarrow 6s10d_{5/2}$	0.0003
	$6s5p_{1/2} \rightarrow 7s10d_{3/2}$	-0.0004	$7s4d_{3/2} \rightarrow 6s8f_{5/2}$	0.0003
	$6s5p_{3/2} \rightarrow 7s10d_{3/2}$	-0.0002	$7s4d_{3/2} \rightarrow 6s9f_{5/2}$	0.0005
	$6s5p_{3/2} \rightarrow 7s8d_{5/2}$	-0.0003	$7s4d_{5/2} \rightarrow 6s8f_{7/2}$	0.0004
	$6s5p_{3/2} \rightarrow 7s9d_{5/2}$	-0.0013	$7s4d_{5/2} \rightarrow 6s8f_{7/2}$	0.0004
	$6s5p_{3/2} \rightarrow 7s10d_{5/2}$	-0.0012	$7s4d_{5/2} \rightarrow 6s9f_{7/2}$	0.0009
	$6s4d_{3/2} \rightarrow 7s8f_{5/2}$	-0.0001		
	$6s4d_{3/2} \rightarrow 7s9f_{5/2}$	-0.0004		
	$6s4d_{5/2} \rightarrow 7s8f_{7/2}$	-0.0005		

corresponding corrections from the normalization of the wave functions to various RCC operators, we get contributions as 0.0018, -0.8980 and 0.0073 from the core correlation, singly excited states and doubly excited states, respectively, in Cs. Similarly, we get the contributions as 0.0271, -14.7551 and 0.3158 from the core correlation, singly excited states and doubly excited states, respectively, in Fr. Clearly, the core correlation and doubly excited states contributions in Fr are large. In Cs and Fr, the doubly excited states contributions are around 1% and 2%, respectively, with opposite signs. Hence, these contributions should also be accounted accurately for high precision results.

To understand more clearly about the role of different excited states that play important roles in the $E1_{PNC}$ result of Cs through our RCC approach which have also been studied by other methods, we consider some of the important RCC terms and analyze their contributions through various excitations level. These results are given explicitly in Table IV. As noticed, only $4p_{1/2}$ and $5p_{1/2}$ core orbitals are important to account the core correlation effects; this is because the single particle energy levels between these orbitals with the valence electrons are small. The singly excited states from $6p_{1/2}$ to $9p_{1/2}$ contribute predominantly, but there are also significant contributions from some of

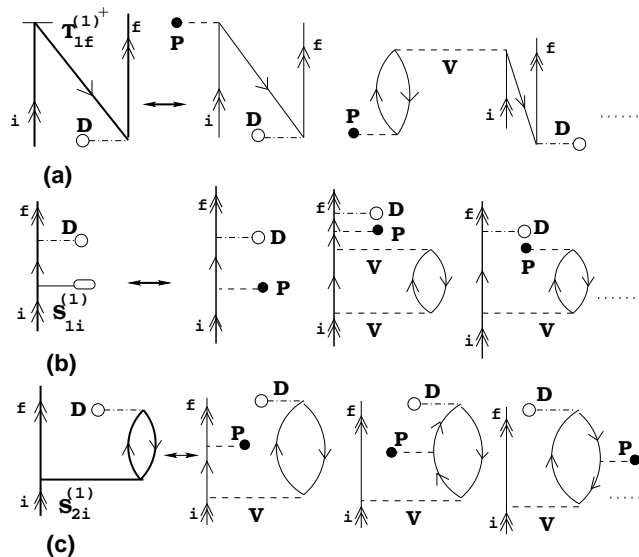


FIG. 2: Break-down of the perturbed RCC diagrams into the lower-order many-body theory (MBPT) diagrams. Here i and f represent the initial and final orbitals, P is the PNC operator and V is the two-body part of the Coulomb interaction Hamiltonian. Lines going up and down with single arrows represent virtual and hole (core) orbitals and lines with double arrows represent attached valence orbitals to the closed-shell DF wave function.

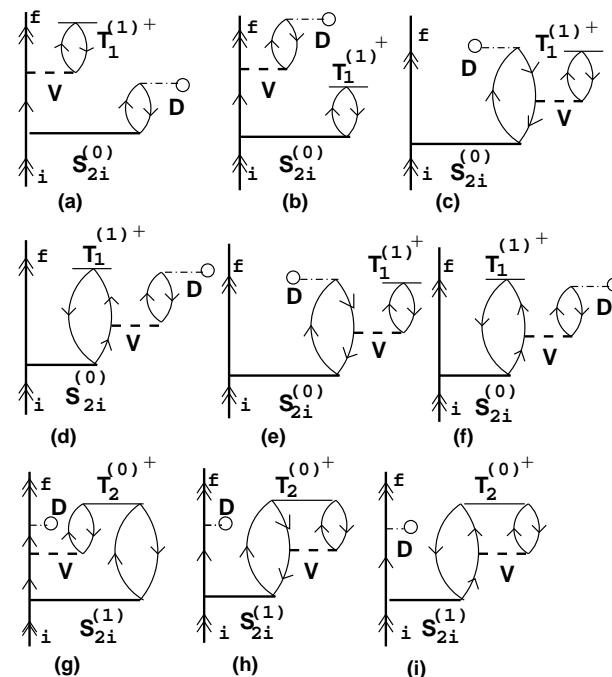


FIG. 3: Some of the important contributing diagrams from the triple excitations which contribute significantly to the lo-CCSDvT method along with their conjugate terms.

the continuum states. The continuum orbital, $10p_{1/2}$, whose density in the nuclear region is large. There are various doubly excited states that play important roles, mainly from the $6skp$ to $7sld$ and $7skp$ to $6sld$ excitations for any arbitrary principal quantum numbers k and l , in calculating the above quantities but mostly they cancel each other. Therefore, a suitable choice of basis functions and an accurate many-body method are necessary for accounting these contributions precisely.

To compare the role of the correlation effects in calculating $E1_{PNC}$ amplitudes in Cs and Fr, we compare the DF results and then their final results. It is about 20% in Cs, but it is only about 7% in Fr. The small correlation

effects in Fr is because of strong cancellations between the contributions from the initial and final perturbed states. Again, it is interesting to note that the CCSD results were larger than the CCSD(T) results suggesting that there were cancellations from the triple excitations. Using the lo-CCSDvT method, these results increase in Cs slightly but cancel out in Fr. The triple excitation effects in Fr are strong enough to be taken seriously into account for high precision results. In Fig. 3, we give some of the important RCC diagrams (without their conjugate terms) that give large contributions through the lo-CCSDvT method. In the future, we would like to study other relevant properties in order to determine the accuracy of our calculated $E1_{PNC}$ amplitudes in these systems.

V. CONCLUSION

We have applied the relativistic coupled-cluster method to calculate the atomic parity violating effects in Cs and Fr which involve the interplay of the long range electrostatic interactions and the short range weak interactions. The present approach considers the Coulomb interaction up to all orders and the weak interaction between the nucleus and the electrons up to first order. From the detailed analysis of different contributions, it is clear that the doubly excited states play an important role in obtaining precise results. These contributions are quite large in magnitude, however, with opposite signs, than those of the singly excited states in Fr, resulting in a large cancellation in the final results. They are about 1% in Cs, for which the experimental accuracies have been claimed to be around 0.35%. This suggests that, it requires a method like our present approach to consider them accurately for high precision calculations.

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- [1] Mohapatra R N and Pati J C 1975 *Phys. Rev. D* **11** 566
 - [2] Barr S M 1993 *Phys. Rev. D* **47** 2025
1992 *Phys. Rev. Lett.* **68** 1822
1992 *Phys. Rev. D* **45** 4148
 - [3] Liu J 1986 *Nucl. Phys. B* **271** 531
 - [4] Ginges J S M and Flambaum V V 2004 *Phys. Rep.* **637** 63
 - [5] Bouchiat M -C, Guéna J and Pottier L 1984 *J. Phys. (France) Lett.* **45** L523
 - [6] Wood C S, Bennett S C, Cho D, Masterson B P, Roberts J L, Tanner C E and Wieman C E 1997 *Science* **275** 1759
 - [7] Vetter P A, Meekhof D M, Majumder P K, Lamoreaux S K and Fortson E N 1995 *Phys. Rev. Lett.* **74** 2658
 - [8] Sahoo B K, Chaudhuri R, Das B P and Mukherjee D 2006 *Phys. Rev. Lett.* **96** 163003
 - [9] Wansbeek L W, Sahoo B K, Timmermans R G, Jungmann K, Das B P and Mukherjee D 2008 *Phys. Rev. A* **78** 050501
 - [10] Anthony P L et al (SLAC E158 Collaboration) 2005 *Phys. Rev. Lett.* **95** 081601
 - [11] Sur C, Latha K V P, Sahoo B K, Chaudhuri R K, Das B P and Mukherjee D 2006 *Phys. Rev. Lett.* **96** 193001
 - [12] Sahoo B K 2007 *Chem. Phys. Lett* **448** 144
 - [13] Blundell S A, Sapirstein J and Johnson W R 1992 *Phys. Rev. D* **45** 1602
 - [14] Dzuba V A, Flambaum V V and Ginges J S M 2002 *Phys. Rev. D* **66** 076013
 - [15] Shabaev V M, Tupitsyn I I, Pachucki K, Plunien G and Yerokhin V A 2005 *Phys. Rev. A* **72** 062105
 - [16] Das B P, Sahoo B K, Gopakumar G and Chaudhuri R K 2006 *J. of Mol. Str. THEOCHEM* **768** 141
 - [17] Dzuba V A, Flambaum V V and Safronova M S 2006 *Phys. Rev. A* **73** 022112
 - [18] Porsev S G, Beloy K and Derevianko A 2009 *Phys. Rev. Lett.* **102** 181601
 - [19] Dzuba V A, Flambaum V V and Sushkhov O P 1995 *Phys. Rev. A* **51** 3454
 - [20] Safronova M S and Johnson W R 2000 *Phys. Rev. A* **62** 022112